Positivity-preserving Lagrangian schemes for multi-material compressible flows

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Joint work with Chi-Wang Shu
Outline

- Introduction
- The positivity-preserving HLLC numerical flux for the Lagrangian method
- The high order positivity-preserving Lagrangian schemes
- Numerical results
- Concluding remarks
I. Introduction
Multi-material problems

Inertial Confinement Fusion

Astrophysics

Underwater explosion

Heavy $\rho_1$

Light $\rho_2$
Methods to Describe Fluid Flow

- **Eulerian Method**
  The fluid flows through a grid fixed in space

- **Lagrangian Method**
  The grid moves with the local fluid velocity

- **ALE Method**
  (Arbitrary Lagrangian-Eulerian )
  The grid motion can be chosen arbitrarily
The Lagrangian Method

- Can capture the material interface automatically
- Can maintain good resolution during large scale compressions/expansions
- Is widely used in many fields for multi-material flow simulations
  
  Astrophysics,
  Inertial Confinement Fusion (ICF),
  Computational fluid dynamics (CFD)

……
The property of positivity-preserving for the numerical method

- As one mathematical aspect of scheme robustness, the positivity-preserving property becomes more and more important for the simulation of fluid flow.

- At high Mach numbers or for flows near vacuum, solving the conservative Euler equations may lead to negative density or internal energy.

- This difficulty is particularly profound for high order methods, for multi-material flows and for problems with moving meshes, such as the Lagrangian method.
The positivity-preserving Eulerian method

- **low order schemes**
  - Godunov scheme
  - The modified HLLE scheme
  - Lax-Friedrichs scheme
  - HLLC scheme
  - AUSM+ scheme
  - Gas-kinetic schemes
  - Flux vector splitting schemes

- **high order schemes** (Zhang & Shu et al.)
  - Runge-Kutta discontinuous Galerkin (RKDG) schemes
  - weighted essentially non-oscillatory (WENO) finite volume schemes
  - WENO finite difference schemes

Up to now, no positivity-preserving Eulerian schemes have involved multi-material problems.
The positivity-preserving Lagrangian method

- The Godunov-type Lagrangian scheme based on the modified HLL Riemann solver
- The positive and entropic Lagrangian schemes for gas dynamics and MHD.

- only first order accurate.
- only valid in 1D space.
- impossible to be extended to higher dimensional space due to the usage of mass coordinate.
The positivity-preserving Lagrangian schemes for multi-material flow

We will discuss the methodology to construct the positivity-preserving Lagrangian schemes. We will propose

- a positivity-preserving HLLC approximate Riemann solver for the Lagrangian schemes
- a class of positivity-preserving Lagrangian schemes
  - 1st order & high order
  - 1D & 2D
  - multi-material flow
  - general equation of state (EOS)
II. The positivity-preserving HLLC numerical flux for the Lagrangian method
The compressible Euler equations in Lagrangian formulation

\[ \frac{d}{dt} \int_{\Omega(t)} U d\Omega + \int_{\Gamma(t)} F d\Gamma = 0 \]

where \( \Omega(t) \) is the moving control volume enclosed by its boundary \( \Gamma(t) \).

\[ U = \begin{pmatrix} \rho \\ M \\ E \end{pmatrix}, \quad F = \begin{pmatrix} 0 \\ \rho \cdot n \\ \rho u \cdot n \end{pmatrix} \]

**Equation of State (EOS)**

\[ p = p(\rho, e) \]

1) The ideal EOS for the ideal gas,
\[ p = (\gamma - 1) \rho e \]

2) The stiffened EOS for water,
\[ p = (\gamma - 1) \rho e - \gamma p_c \]

3) The Jones-Wilkins-Lee (JWL) EOS for the detonation-products gas,
\[ p = (\gamma - 1) \rho e + f(\rho) \]
\[ f(\rho) = A_1(1 - \frac{\omega \rho}{R_1 \rho_0}) e^{-\frac{R_1 \rho_0}{\rho}} + A_2(1 - \frac{\omega \rho}{R_2 \rho_0}) e^{-\frac{R_2 \rho_0}{\rho}} \]
The general form of the cell-centered Lagrangian schemes

\[ \overline{U}_{i}^{n+1} \Delta x_{i}^{n+1} - \overline{U}_{i}^{n} \Delta x_{i}^{n} = -\Delta t \left[ \hat{F}(\overline{U}_{i+1/2}^{-}, \overline{U}_{i+1/2}^{+}) - \hat{F}(\overline{U}_{i-1/2}^{-}, \overline{U}_{i-1/2}^{+}) \right] \]

\[ \overline{U} = \begin{pmatrix} \rho \\ \frac{m}{E} \end{pmatrix}, \quad \hat{F} = \begin{pmatrix} \hat{f}_{D} \\ \hat{f}_{N} \end{pmatrix} \]

The left and right values of the primitive variables on each side of the boundary
- 1st order: \( \overline{U} \)
- High order: reconstruction

The first order scheme

\[ \overline{U}_{i}^{n+1} \Delta x_{i}^{n+1} = \overline{U}_{i}^{n} \Delta x_{i}^{n} - \Delta t \left[ \hat{F}(\overline{U}_{i}^{n}, \overline{U}_{i+1}^{n}) - \hat{F}(\overline{U}_{i-1}^{n}, \overline{U}_{i}^{n}) \right] \]
The HLLC numerical flux for the Lagrangian scheme

\[
\begin{aligned}
    \frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} &= 0 \\
    U(x, 0) &= \begin{cases} 
        U^-, & x < 0 \\
        U^+, & x \geq 0.
    \end{cases}
\end{aligned}
\]

\[
\hat{F}(U^-, U^+) = F(U^*) = \begin{pmatrix} 0 \\ p^* \\ p^* S_* \end{pmatrix}
\]

the similarity solution along the contact wave

\[
p^* = \rho_-(u_- - S_-)(u_- - S_m) + p_-
\]

\[
S_* = \frac{\rho_+ u_+(S_+ - u_+) - \rho_- u_-(S_- - u_-) + p_- - p_+}{\rho_+(S_+ - u_+) - \rho_-(S_- - u_-)}
\]
The choice of left and right acoustic wave speeds

\[ \{ \overline{U}_i^n \in G, i = 1, \ldots, N \} \Rightarrow \{ \overline{U}_i^{n+1} \in G, i = 1, \ldots, N \} \]

- divergence theorem
- G is a convex set
- Jensen's inequality for integrals

\[ U_{\pm} \in G \Rightarrow U_{\pm}^* \in G \]

\[ S_- = \min \left[ u_- - \frac{p_-}{\rho_- \sqrt{2e_-}}, u_- - c_-, \tilde{u} - \tilde{c} \right] \]
\[ S_+ = \max \left[ u_+ + \frac{c_+}{\rho_+ \sqrt{2e_+}}, u_+ + c_+, \tilde{u} + \tilde{c} \right] \]

\[ G = \left\{ U = \begin{bmatrix} \rho \\ \rho u \end{bmatrix}, \rho > 0, \ e = E/\rho - \frac{1}{2} |u|^2 > 0, \ c^2 = p_p |s| > 0 \right\} \]
The first order positivity preserving Lagrangian scheme in 1D space

**Theorem:**

The first order Lagrangian scheme for Euler equations with the general EOS in 1D space is **positivity-preserving** if the acoustic wavespeeds $S_-$ and $S_+$ and the time step restriction are satisfied:

\[
S_- = \min\{u_- - \frac{p_-}{\rho_- \sqrt{2e_-}}, u_- - c_-, \tilde{u} - \tilde{c}\}, \quad S_+ = \max\{u_+ + \frac{p_+}{\rho_+ \sqrt{2e_+}}, u_+ + c_+, \tilde{u} + \tilde{c}\}
\]

\[
\Delta t^n \leq \lambda \min_{i=1,...,N} \left( \frac{\Delta x_i^n}{\left( \max \left\{ \left| \frac{p_i^n}{\rho_i^n \sqrt{2e_i^n}} \right|, c_i^n \right\} + |u_i^n| \right)} \right)
\]

\[
\lambda = \frac{1}{2}
\]
The general form for 2D Lagrangian schemes

\[ \bar{U}_{i,j}^n A_{i,j}^{n+1} - \bar{U}_{i,j}^n A_{i,j}^n = -\Delta t \int_{\partial I_{i,j}} \hat{F}(U^{\text{int}(I_{i,j})}, U^{\text{ext}(I_{i,j})}, n_{I_{i,j}}) dl \]

\[ \bar{U}_{i,j} = \begin{pmatrix} \bar{\rho}_{i,j} \\ \bar{m}_{i,j} \\ \bar{E}_{i,j} \end{pmatrix}, \quad \hat{F} = \begin{pmatrix} \hat{f}_D \\ \hat{f}_m \\ \hat{f}_E \end{pmatrix} \]

\[ \hat{f}_D = \rho^\text{int}(u^\text{int}_n - S_-)(u^\text{int}_n - S_+) + p^\text{int}, \]

\[ \hat{f}_m = \rho^\text{int}u^\text{int}_n(S_+ - u^\text{ext}_n) - \rho^\text{int}u^\text{int}_n(S_- - u^\text{int}_n) + p^\text{int} - p^\text{ext} \]

\[ \hat{f}_E = \frac{\rho^\text{ext}u^\text{ext}_n(S_+ - u^\text{ext}_n) - \rho^\text{int}u^\text{int}_n(S_- - u^\text{int}_n)}{\rho^\text{ext}(S_+ - u^\text{ext}_n) - \rho^\text{int}(S_- - u^\text{int}_n)} \]
Theorem:

The 2D first order positivity-preserving Lagrangian scheme is **positivity-preserving** if the acoustic wavespeeds $S_{-}$ and $S_{+}$ and the time step restriction are satisfied:

\[
S_{-} = \min \left[ u_{n}^{\text{int}} - \frac{p_{n}^{\text{int}}}{\rho_{n}^{\text{int}} \sqrt{2 c_{n}^{\text{int}}}}, u_{n}^{\text{int}} - c_{n}^{\text{int}}, \tilde{u}_{n} - \tilde{c} \right]
\]

\[
S_{+} = \max \left[ u_{n}^{\text{ext}} + \frac{p_{n}^{\text{ext}}}{\rho_{n}^{\text{ext}} \sqrt{2 c_{n}^{\text{ext}}}}, u_{n}^{\text{ext}} + c_{n}^{\text{ext}}, \tilde{u}_{n} + \tilde{c} \right]
\]

\[
\Delta t^{n} \leq \lambda \min_{i,j} \left\{ \frac{A_{i,j}^{n}}{\sum_{m=1}^{M} l_{i,j}^{m}} \left( \max \left\{ \left| \frac{p_{i,j}^{n}}{\rho_{i,j}^{n} \sqrt{2 c_{i,j}^{n}}} \right|, c_{i,j}^{n} \right\} + |u_{i,j}^{n}| \right) \right\}
\]

$\lambda = 1/2$
III. The high order positivity-preserving Lagrangian schemes
The high order positivity-preserving Lagrangian scheme in 1D space

\[ \bar{U}_{i}^{n+1} \Delta x_{i}^{n+1} - \bar{U}_{i}^{n} \Delta x_{i}^{n} = -\Delta t [\hat{F}(U_{i+1/2}^{-}, U_{i+1/2}^{+}) - \hat{F}(U_{i-1/2}^{-}, U_{i-1/2}^{+})] \]

(Euler forward time discretization)

Consider the $K$-point Legendre Gauss-Lobatto quadrature rule on the interval $I_i$

\[ S_i = \{ x_{i-\frac{1}{2}} = \hat{x}_i^1, \hat{x}_i^2, \ldots, \hat{x}_i^{K-1}, \hat{x}_i^K = x_{i+\frac{1}{2}} \} \]

\[ \bar{U}_{i}^{n} = \frac{1}{\Delta x_{i}} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} U_i(x) dx = \sum_{\alpha=1}^{K} \omega_{\alpha} U_i(\hat{x}_i^{\alpha}) = \sum_{\alpha=2}^{K-1} \omega_{\alpha} U_i(\hat{x}_i^{\alpha}) + \omega_1 U_{i-1/2}^{+} + \omega_K U_{i+1/2}^{-} \]
\[ \overline{U}_i^{n+1} \Delta x_i^{n+1} = \sum_{\alpha=1}^{K} \omega_\alpha U_i^n \Delta x_i^n - \Delta t [\hat{F}(U_{i+\frac{1}{2}}^-, U_{i+\frac{1}{2}}^+) - \hat{F}(U_{i-\frac{1}{2}}^+, U_{i-\frac{1}{2}}^-) + \hat{F}(U_{i-\frac{1}{2}}^+, U_{i+\frac{1}{2}}^-) - \hat{F}(U_{i-\frac{1}{2}}^-, U_{i+\frac{1}{2}}^-)] - \sum_{\alpha=2}^{K-1} \omega_\alpha U_i^n \Delta x_i^n \\
+ \omega_K \{U_{i+\frac{1}{2}}^- \Delta x_i^n - \frac{\Delta t}{\omega_K} [\hat{F}(U_{i+\frac{1}{2}}^-, U_{i+\frac{1}{2}}^+) - \hat{F}(U_{i-\frac{1}{2}}^+, U_{i+\frac{1}{2}}^-)]\} \\
+ \omega_1 \{U_{i-\frac{1}{2}}^+ \Delta x_i^n - \frac{\Delta t}{\omega_1} [\hat{F}(U_{i-\frac{1}{2}}^+, U_{i+\frac{1}{2}}^-) - \hat{F}(U_{i-\frac{1}{2}}^-, U_{i+\frac{1}{2}}^+)]\} \\
= \sum_{\alpha=2}^{K-1} \omega_\alpha U_i^n \Delta x_i^n + \omega_K \hat{F}_K + \omega_1 \hat{F}_1 \]

where
\[
\hat{F}_1 = U_{i-\frac{1}{2}}^+ \Delta x_i^n - \frac{\Delta t}{\omega_1} [\hat{F}(U_{i-\frac{1}{2}}^-, U_{i+\frac{1}{2}}^+) - \hat{F}(U_{i-\frac{1}{2}}^+, U_{i-\frac{1}{2}}^-)], \\
\hat{F}_K = U_{i+\frac{1}{2}}^- \Delta x_i^n - \frac{\Delta t}{\omega_K} [\hat{F}(U_{i+\frac{1}{2}}^-, U_{i+\frac{1}{2}}^+) - \hat{F}(U_{i+\frac{1}{2}}^+, U_{i-\frac{1}{2}}^-)].
\]

1st order scheme:
\[
\overline{U}_i^{n+1} \Delta x_i^{n+1} = \overline{U}_i^n \Delta x_i^n - \Delta t [\hat{F}(\overline{U}_i^n, \overline{U}_{i+1}^n) - \hat{F}(\overline{U}_i^n, \overline{U}_{i-1}^n)]
\]
Theorem:

The 1D high order Lagrangian scheme is positivity-preserving if it uses the above described HLLC flux and satisfies:

the sufficient condition:

\[
\mathbf{U}_i(\hat{x}_i^\alpha) \in G, \quad \forall \hat{x}_i^\alpha \in S_i, \quad \alpha = 1, \ldots, K
\]

the time step restriction:

\[
\Delta t^n \leq \lambda \omega_1 \min_{i,\alpha} \left( \frac{\Delta x_i^n}{\max \left\{ \left| \frac{p_i^\alpha}{\rho_i^\alpha \sqrt{2c_i^\alpha}} \right|, c_i^\alpha \right\} + |u_i^\alpha|} \right)
\]
The positivity-preserving limiter for the high order Lagrangian scheme

- Firstly, enforce the positivity of density,
  \[ \hat{\rho}_i(x) = \theta^1_i [\rho_i(x) - \bar{\rho}_i] + \bar{\rho}_i, \quad \theta^1_i = \min_{x \in S_i} \left\{ 1, \frac{\bar{\rho}_i - \varepsilon}{\bar{\rho}_i - \rho_i(x)} \right\} \]
  \[ \hat{U}_i = (\hat{\rho}_i, m_i, E_i)^T \]

- Secondly
  - enforce the positivity of internal energy \( e \) for the cells with the ideal EOS or the JWL EOS,
    \[
    \text{if } e(\hat{U}_i(x)) \geq 0 \text{ set } \theta_x = 1; \quad \text{otherwise, set } \theta_x = \frac{e(\hat{U}_i)}{e(\hat{U}_i) - e(\hat{U}_i(x))}
    \]
  - enforce the positivity of \( \tilde{e} = \rho e - p_c \) for the cells with the stiffened EOS,
    \[
    \text{if } \tilde{e}(\hat{U}_i(x)) \geq 0 \text{ set } \theta_x = 1; \quad \text{otherwise, set } \theta_x = \frac{\tilde{e}(\hat{U}_i)}{\tilde{e}(\hat{U}_i) - \tilde{e}(\hat{U}_i(x))}
    \]

- Finally
  \[ \tilde{U}_i(x) = \theta^2_i (\hat{U}_i(x) - \hat{U}_i) + \hat{U}_i, \quad \theta^2_i = \min_{x \in S_i} \theta_x \]

This limiter can keep accuracy, conservation and positivity.
The high order time discretization for the Lagrangian scheme

The TVD Runge-Kutta method

At each Runge-Kutta step, we need to update:

- conserved variables
- vertex velocity
- position of the vertex
- size of the cell
The third order TVD Runge-Kutta method

\[ x_{i-1/2}^{(1)} = x_{i-1/2}^n + u_{i-1/2}^n \Delta t^n, \quad \Delta x_i^{(1)} = x_{i-1/2}^{(1)} - x_{i-1/2}^{(1)} \]

\[ \bar{U}_i^{(1)} \Delta x_i^{(1)} = \bar{U}_i^n \Delta x_i^n + \Delta t^n L(\bar{U}_i^n); \]

\[ x_{i-1/2}^{(2)} = \frac{3}{4} x_{i-1/2}^n + \frac{1}{4} [x_{i-1/2}^{(1)} + u_{i-1/2}^{(1)} \Delta t^n], \quad \Delta x_i^{(2)} = x_{i-1/2}^{(2)} - x_{i-1/2}^{(2)} \]

\[ \bar{U}_i^{(2)} \Delta x_i^{(2)} = \frac{3}{4} \bar{U}_i^n \Delta x_i^n + \frac{1}{4} [\bar{U}_i^{(1)} \Delta x_i^{(1)} + \Delta t^n L(\bar{U}_i^{(1)})]; \]

\[ x_{i-1/2}^{n+1} = \frac{1}{3} x_{i-1/2}^n + \frac{2}{3} [x_{i-1/2}^{(2)} + u_{i-1/2}^{(2)} \Delta t^n], \quad \Delta x_i^{n+1} = x_{i-1/2}^{n+1} - x_{i-1/2}^{n+1} \]

\[ \bar{U}_i^{n+1} \Delta x_i^{n+1} = \frac{1}{3} \bar{U}_i^n \Delta x_i^n + \frac{2}{3} [\bar{U}_i^{(2)} \Delta x_i^{(2)} + \Delta t^n L(\bar{U}_i^{(2)})] \]
The high order positivity-preserving Lagrangian scheme in 2D

The scheme with the Euler forward time discretization

\[
\frac{\mathbf{U}^{n+1}_{i,j} - \mathbf{U}^n_{i,j}}{\Delta t} = - \Delta t \sum_{m=1}^{4} \sum_{\alpha=1}^{K} \omega_{\alpha} \hat{F}(\mathbf{U}^{\text{int}}_{m,\alpha}(I_{i,j}), \mathbf{U}^{\text{ext}}_{m,\alpha}(I_{i,j}), n_{i,j}^m) l_{i,j}^m
\]

- ENO reconstruction
- Numerical flux
  - The HLLC flux
- Gaussian integration for the line integral
The Gauss-Lobatto quadrature for the polynomials in cells with general quadrilateral shape

\[
\overline{U}_{i,j}^n = \frac{1}{A_{i,j}^n} \int_{I_{i,j}} \int_{I_{i,j}} U_{i,j}(x, y) dxdy
\]

\[
= \frac{1}{A_{i,j}^n} \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} U_{i,j}(g_{i,j}(\xi, \eta)) \left. \frac{\partial g_{i,j}(\xi, \eta)}{\partial (\xi, \eta)} \right|_{(\xi, \eta)} d\xi d\eta
\]

\[
= \frac{1}{A_{i,j}^n} \sum_{\alpha=1}^{K} \sum_{\beta=1}^{K} \omega_\alpha \omega_\beta U_{i,j}(g_{i,j}(\xi_\alpha, \eta_\beta)) \left. \frac{\partial g_{i,j}(\xi, \eta)}{\partial (\xi, \eta)} \right|_{(\xi_\alpha, \eta_\beta)}
\]

\[
= \frac{1}{A_{i,j}^n} \sum_{\alpha=1}^{K} \sum_{\beta=1}^{K} \omega_\alpha \omega_\beta \left. \frac{\partial g_{i,j}(\xi, \eta)}{\partial (\xi, \eta)} \right|_{(\xi_\alpha, \eta_\beta)} U_{i,j}^{\alpha, \beta}
\]
The design of 2D high order positivity-preserving Lagrangian scheme

\[
\overline{U}_{i,j}^{n+1} A_{i,j}^{n+1} = \frac{1}{2} \left[ \sum_{\beta=2}^{K-1} \sum_{\alpha=1}^{K} \tilde{\omega}_{\beta \alpha} U_{i,j}^{\beta \alpha} + \sum_{\beta=2}^{K-1} \sum_{\alpha=1}^{K} \tilde{\omega}_{\alpha \beta} U_{i,j}^{\alpha \beta} \right] \\
+ \frac{1}{2} \omega_1 \sum_{\alpha=1}^{K} \omega_{\alpha} \left[ U_{1,\alpha}^{\text{int}(I_{i,j})} |J|_{i,j}^{1,\alpha} + U_{2,\alpha}^{\text{int}(I_{i,j})} |J|_{i,j}^{1,\alpha} + U_{3,\alpha}^{\text{int}(I_{i,j})} |J|_{i,j}^{1,\alpha} + U_{4,\alpha}^{\text{int}(I_{i,j})} |J|_{i,j}^{1,\alpha} \right] \\
- \Delta t \sum_{m=1}^{4} \sum_{\alpha=1}^{K} \omega_{\alpha} \hat{F}(U_{m,\alpha}^{\text{int}(I_{i,j})}, U_{m,\alpha}^{\text{ext}(I_{i,j})}, n_{I_{i,j}}^{m}) |l_{i,j}^{m}| \\

By adding and subtracting \( \Delta t \hat{F}(U_{1,\alpha}^{\text{int}(I_{i,j})}, U_{m,\alpha}^{\text{int}(I_{i,j})}, n_{I_{i,j}}^{m}) |l_{i,j}^{m}|, m = 2, 4 \)

\[
\overline{U}_{i,j}^{n+1} A_{i,j}^{n+1} = \frac{1}{2} \left[ \sum_{\beta=2}^{K-1} \sum_{\alpha=1}^{K} \tilde{\omega}_{\beta \alpha} U_{i,j}^{\beta \alpha} + \sum_{\beta=2}^{K-1} \sum_{\alpha=1}^{K} \tilde{\omega}_{\alpha \beta} U_{i,j}^{\alpha \beta} \right] \\
+ \frac{1}{2} \omega_1 \sum_{\alpha=1}^{K} \omega_{\alpha} \left[ \hat{F}_{\alpha}^{1} + \hat{F}_{\alpha}^{2} + \hat{F}_{\alpha}^{3} + \hat{F}_{\alpha}^{4} \right] \\
|J|_{i,j}^{1,\alpha} = \frac{\partial g_{i,j}(\xi,\eta)}{\partial (\xi,\eta)} |(\xi,\eta)|, \tilde{\omega}_{\alpha \beta} = \omega_0 \omega_\beta |J|_{i,j}^{1,\alpha} 
\]
where

\[ \hat{F}_1^i = \frac{\partial_t}{\partial x} \left[ F(U_{1,\alpha}^{int(I_{i,j})}, U_{1,\alpha}^{ext(I_{i,j})}, n_{i,j}^{1}) \right] + \hat{F}(U_{1,\alpha}^{int(I_{i,j})}, U_{2,\alpha}^{int(I_{i,j})}, n_{i,j}^{2}) \]

\[ + \hat{F}(U_{1,\alpha}^{int(I_{i,j})}, U_{3,\alpha}^{int(I_{i,j})}, n_{i,j}^{3}) + \hat{F}(U_{1,\alpha}^{int(I_{i,j})}, U_{4,\alpha}^{int(I_{i,j})}, n_{i,j}^{4}) \]

\[ \hat{F}_2^i = \frac{\partial_t}{\partial x} \left[ F(U_{2,\alpha}^{int(I_{i,j})}, U_{2,\alpha}^{ext(I_{i,j})}, n_{i,j}^{1}) \right] - \hat{F}(U_{1,\alpha}^{int(I_{i,j})}, U_{2,\alpha}^{int(I_{i,j})}, n_{i,j}^{2}) \]

\[ \hat{F}_3^i = \frac{\partial_t}{\partial x} \left[ F(U_{3,\alpha}^{int(I_{i,j})}, U_{3,\alpha}^{ext(I_{i,j})}, n_{i,j}^{1}) \right] - \hat{F}(U_{1,\alpha}^{int(I_{i,j})}, U_{3,\alpha}^{int(I_{i,j})}, n_{i,j}^{2}) \]

\[ \hat{F}_4^i = \frac{\partial_t}{\partial x} \left[ F(U_{4,\alpha}^{int(I_{i,j})}, U_{4,\alpha}^{ext(I_{i,j})}, n_{i,j}^{1}) \right] - \hat{F}(U_{1,\alpha}^{int(I_{i,j})}, U_{4,\alpha}^{int(I_{i,j})}, n_{i,j}^{2}) \]

a formal 2D first order positivity-preserving scheme

\[ \hat{F}_2^i, \hat{F}_3^i \] and \[ \hat{F}_4^i \]

formal 1D first order positivity-preserving schemes

- The positivity-preserving limiter is performed on \( U_{i,j}(x, y) \) to make \( U_{i,j}^{\alpha,\beta} \in G \).
- The TVD Runge-Kutta method is used for the high order time discretization.
The high order positivity-preserving Lagrangian scheme in 2D

Theorem:

The 2D high order Lagrangian scheme is \textit{positivity-preserving} if it uses the above described HLLC flux and satisfies:

the sufficient condition:

\[ U_{i,j}^{\alpha,\beta} \in G, \ \forall \alpha, \beta = 1, K; i = 1, ..., M, j = 1, ..., N \]

the time step restriction:

\[ \Delta t^n \leq \frac{\omega_1}{2} \lambda \min_{i,j,\alpha,\beta} \left\{ \frac{|J|_{i,j}}{\sum_{m=1,4}^{m} f_{i,j}} \right\} \left( \max \left\{ \left| \frac{p_{i,j}^{\alpha,\beta}}{\rho_{i,j}^{\alpha,\beta} \sqrt{2c_{i,j}^{\alpha,\beta}}} \right|, c_{i,j}^{\alpha,\beta} \right\} + |u_{i,j}^{\alpha,\beta}| \right) \]
IV. Numerical results

- 1D case

- 2D case

All the numerical examples shown here can’t be simulated by the general high order Lagrangian schemes without the positivity-preserving limiter successfully.
1D Numerical tests

1. The isentropic smooth problem (accuracy test)

The initial condition:

\[ \rho(x, 0) = 1 + 0.999995 \sin(\pi x), \quad u(x, 0) = 0, \quad p(x, 0) = \rho^\gamma(x, 0), \quad x \in [-1, 1] \]

time=0.1
Errors for the 1st order positivity-preserving Lagrangian scheme

<table>
<thead>
<tr>
<th>$N_x$</th>
<th>Norm</th>
<th>Density</th>
<th>order</th>
<th>Momentum</th>
<th>order</th>
<th>Energy</th>
<th>order</th>
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<td>100</td>
<td>$L_1$</td>
<td>0.94E-2</td>
<td></td>
<td>0.29E-1</td>
<td></td>
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<td></td>
<td>$L_\infty$</td>
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<td>0.65E-1</td>
<td></td>
<td>0.72E-1</td>
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<td>200</td>
<td>$L_1$</td>
<td>0.48E-2</td>
<td>0.97</td>
<td>0.15E-1</td>
<td>0.96</td>
<td>0.14E-1</td>
<td>0.95</td>
</tr>
<tr>
<td></td>
<td>$L_\infty$</td>
<td>0.11E-1</td>
<td>0.95</td>
<td>0.33E-1</td>
<td>0.96</td>
<td>0.38E-1</td>
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<td>400</td>
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<td>0.24E-2</td>
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<td>0.98</td>
<td>0.17E-1</td>
<td>0.98</td>
<td>0.19E-1</td>
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</tr>
<tr>
<td>800</td>
<td>$L_1$</td>
<td>0.12E-2</td>
<td>0.99</td>
<td>0.38E-2</td>
<td>0.99</td>
<td>0.35E-2</td>
<td>0.99</td>
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<td>0.86E-2</td>
<td>0.99</td>
<td>0.99E-2</td>
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</table>
Errors for the 3rd order positivity-preserving Lagrangian scheme

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<th>$N_x$</th>
<th>Norm</th>
<th>Density</th>
<th>order</th>
<th>Momentum</th>
<th>order</th>
<th>Energy</th>
<th>order</th>
<th>limited cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>$L_1$</td>
<td>0.11E-3</td>
<td>0.14E-3</td>
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<td></td>
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<tr>
<td></td>
<td>$L_\infty$</td>
<td>0.85E-3</td>
<td>0.67E-3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>200</td>
<td>$L_1$</td>
<td>0.14E-4</td>
<td>2.94</td>
<td>0.17E-4</td>
<td>3.07</td>
<td>0.18E-4</td>
<td>2.96</td>
<td>1%</td>
</tr>
<tr>
<td></td>
<td>$L_\infty$</td>
<td>0.85E-4</td>
<td>3.32</td>
<td>0.85E-4</td>
<td>2.98</td>
<td>0.78E-4</td>
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</tr>
<tr>
<td>400</td>
<td>$L_1$</td>
<td>0.16E-5</td>
<td>3.07</td>
<td>0.21E-5</td>
<td>3.00</td>
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<td>$L_1$</td>
<td>0.20E-6</td>
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<td>0.27E-6</td>
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<td>$L_\infty$</td>
<td>0.11E-5</td>
<td>3.36</td>
<td>0.13E-5</td>
<td>3.00</td>
<td>0.12E-5</td>
<td>2.99</td>
<td></td>
</tr>
</tbody>
</table>
2. 123 problem

The initial condition:

\begin{align*}
\rho_L &= 1 \\
u_L &= -2 \\
p_L &= 0.4 \\
\gamma_L &= 1.4 \\
\rho_R &= 1 \\
u_R &= 2 \\
p_R &= 0.4 \\
\gamma_R &= 1.4
\end{align*}

- contain vacuum
density
velocity
internal energy

400 cells
time=1.0
Non positivity-preserving & positivity-preserving density pressure internal energy
3. The gas-liquid shock-tube problem

The initial condition:

- \( \rho_L = 5 \)
- \( u_L = 0 \)
- \( p_L = 10^5 \)
- \( \gamma_L = 1.4 \)
- \( \rho_R = 1000 \)
- \( u_R = 0 \)
- \( p_R = 10^9 \)
- \( \gamma_R = 4.4 \)

- multi-material
- strong interfacial contact discontinuity
density
velocity
internal energy

200 cells
time=0.00024
4. The spherical underwater explosion

The initial condition:

\[ \rho_L = 0.00163 \]
\[ u_L = 0. \]
\[ p_L = 8381 \]
\[ \rho_R = 0.00125 \]
\[ u_R = 0. \]
\[ p_R = 1 \]

- multi-material
- general EOS
- large pressure jump
2D Numerical Tests

1. the vortex problem (accuracy test)

The initial condition:

The mean flow: \( p = 1. \rho = 1, (u, v) = (1, 1) \)

Add an isentropic vortex perturbations:

\[
(\delta u, \delta v) = \frac{\epsilon}{2\pi} e^{0.5(1-r^2)}(-\bar{y}, \bar{x})
\]

\[
\delta T = -\frac{(\gamma - 1)\epsilon^2}{8\gamma \pi^2} e^{1-r^2}, \quad \delta S = 0,
\]

where \((\bar{x}, \bar{y}) = (x - 5, y - 5), r^2 = \bar{x}^2 + \bar{y}^2,\) and the vortex strength \(\epsilon = 10.0828\)

lowest density: \(7.8 \times 10^{-15}\)

lowest pressure: \(1.7 \times 10^{-2}\)
Errors for the 1st order positivity-preserving Lagrangian scheme

<table>
<thead>
<tr>
<th>$N_x = N_y$</th>
<th>Norm</th>
<th>Density</th>
<th>order</th>
<th>Momentum</th>
<th>order</th>
<th>Energy</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>$L_1$</td>
<td>0.30E-2</td>
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<td>0.10E-1</td>
<td></td>
<td>0.15E-1</td>
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<tr>
<td></td>
<td>$L_\infty$</td>
<td>0.45E-1</td>
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<td>0.99E-1</td>
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<td>0.29E+0</td>
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<td>$L_1$</td>
<td>0.13E-2</td>
<td>1.25</td>
<td>0.43E-2</td>
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<td>0.68E-2</td>
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<td>0.20E-1</td>
<td>1.15</td>
<td>0.46E-1</td>
<td>1.12</td>
<td>0.13E+0</td>
<td>1.12</td>
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<tr>
<td>80</td>
<td>$L_1$</td>
<td>0.57E-3</td>
<td>1.16</td>
<td>0.20E-2</td>
<td>1.15</td>
<td>0.31E-2</td>
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<tr>
<td></td>
<td>$L_\infty$</td>
<td>0.90E-2</td>
<td>1.16</td>
<td>0.22E-1</td>
<td>1.03</td>
<td>0.61E-1</td>
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<tr>
<td>160</td>
<td>$L_1$</td>
<td>0.27E-3</td>
<td>1.09</td>
<td>0.92E-3</td>
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<td>0.42E-2</td>
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Errors for the 2nd order positivity-preserving Lagrangian scheme

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<th>Norm</th>
<th>Density</th>
<th>order</th>
<th>Momentum</th>
<th>order</th>
<th>Energy</th>
<th>order</th>
<th>limited cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>$L_1$</td>
<td>0.26E-2</td>
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<td>0.73E-2</td>
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<td>1%</td>
</tr>
<tr>
<td></td>
<td>$L_\infty$</td>
<td>0.37E-1</td>
<td></td>
<td>0.93E-1</td>
<td></td>
<td>0.26E+0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>$L_1$</td>
<td>0.73E-3</td>
<td>1.85</td>
<td>0.20E-2</td>
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<tr>
<td></td>
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<td>0.12E-1</td>
<td>1.67</td>
<td>0.27E-1</td>
<td>1.80</td>
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<tr>
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<td>0.19E-3</td>
<td>1.94</td>
<td>0.50E-3</td>
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<tr>
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<td>0.84E-2</td>
<td>1.66</td>
<td>0.22E-1</td>
<td>1.69</td>
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</tr>
<tr>
<td>160</td>
<td>$L_1$</td>
<td>0.48E-4</td>
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<td>0.13E-3</td>
<td>1.98</td>
<td>0.23E-3</td>
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<td>0.12E-2</td>
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<td>1.75</td>
<td>0.68E-2</td>
<td>1.68</td>
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</tr>
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</table>
2. The Sedov blast wave problem

The initial condition (on the domain $1.1 \times 1.1$ with $30 \times 30$ cells):

$$\rho = 1, \quad p = 10^{-14}, \quad u_x = u_y = 0, \quad \gamma = 1.4$$

$$e(1,1) = 182.09$$

The exact solution:

A shock at the radius=1 with a peak density of 6 at the time=1.
3. The air-water-air problem

Initial condition:

\[ (\rho, u, v, p, \gamma, p_c) = \begin{cases} 
(1000, 0, 0, 0.001, 1.4, 0), & 0 \leq r \leq 0.2 \\
(1, 0, 0, 1, 7, 3000), & 0.2 < r \leq 1.0 \\
(0.001, 0, 0, 0.001, 1.4, 0), & 1.0 < r \leq 1.2 
\end{cases} \]
t=0.0015  t=0.003  t=0.007

2nd order

grid
density
velocity

internal energy

t=0.0015  
t=0.003  
t=0.007

2nd order
The cut contour results

density

velocity

internal energy

t=0.0015  
t=0.003  
t=0.007
V. Concluding remarks

We have described the general techniques to construct the positivity-preserving Lagrangian schemes for the compressible Euler equations with the general equation of state both in 1D and 2D space.

- a positivity-preserving HLLC approximate Riemann solver for the Lagrangian scheme.
- a class of first order and high order positivity-preserving Lagrangian schemes.

Future work:
- Generalize the schemes to cylindrical coordinates.
- Improve the robustness of the high order positivity-preserving Lagrangian schemes.
Thanks for your attention!
Reference